with lipid bilayers are described and understood quite well. Recently, new types of detergents with cyclohexyl groups or branches in their hydrophobic tails have been synthesized and proposed to be superior for membrane protein studies. Cymal-6 has, for example, been used for isolating membrane proteins such as CCR5 and HIV-1 corepressors. Here we provide a rather comprehensive description of the interactions of Cymal-6 with fluid membranes of POPC. This includes the temperature-dependent phase behavior (i.e., the onset and completion of solubilization), membrane partitioning, disordering, and permeabilization as seen using ITC, time-resolved fluorescence anisotropy of DPH, dynamic light scattering, and the lifetime-based vesicle leakage assay.

421-Pos Board B190
Characterizing the Interactions of Lysophospholipids with Lipid Membranes
Dew Das, Arpit Shah, Mozhgan Nazari, Hiren Patel, Heiko Heerklotz.
University of Toronto, Toronto, ON, Canada.
This study aims to characterize and compare thermodynamic interactions of the lysophospholipid - C12 - lysophosphocholine (lysoPC) and its synthetic analog, n-dodecylphosphocholine (DPC) - with lipid membranes. As a biomolecule possessing detergent-like properties, lysoPC is involved in many biological processes and DPC has been used widely in NMR studies of membrane proteins. We investigate the lipid-detergent systems by determining partition coefficient, mole ratios of bound detergent to lipid at membrane saturation and solubilization boundaries, and the mechanism of membrane disordering and pore formation. Isothermal Titration Calorimetry (ITC) is used for assays such as demicellization, uptake-and-release and solubilization-and-reconstitution. Time-resolved DPH anisotropy and lifetime-based leakage assays are used to study membrane structural changes upon detergent incorporation in liposomes. Both lysoPC and DPC equilibrate with membranes very slowly. We hypothesize that the free energy penalty due to asymmetric membrane insertion limits the membrane uptake of lysoPC and DPC. This would be at variance to other detergents that induce membrane failure above a threshold asymmetry. Results are important for understanding mechanisms for membrane protein isolation and the interactions of amphiphilic biological compounds with lipid membranes.

422-Pos Board B191
Suppression of Cooperative Motions in Phospholipid Membranes by Osmotic Stress: Deuterium NMR Relaxation Study
Trivikram R. Molugu[1], K.J. Mallikarjunaiah[1], Constantin Job[1], Michael F. Brown[1,2].
[1]Department of Chemistry and Biochemistry, University of Arizona, Tucson, AZ, USA, [2]Department of Physics, University of Arizona, Tucson, AZ, USA.
Understanding membrane dynamics is crucial to explaining the function of membrane proteins. Phospholipids are commonly employed as model systems to investigate biological membranes. The complex dynamic organization of phospholipid membranes spans several frequency decades, starting from subpicosecond local motions to millisecond collective dynamics [1]. Such motional frequencies can be accessed using various NMR relaxation methods. To address membrane dynamics mediated by osmotic stress, we measured ^{2}H longitudinal (R_{1Z}) and transverse quadrupolar echo (R_2^{QE}) relaxation rates for the liquid-crystalline phase of DMPC-d_{54} membrane bilayers. Osmotic stress was applied by both dehydration and osmolyte concentration [2]. The R_{1Z} values of individual acyl segments were independent of osmotic stress while the segmental order parameters (S_{CD}) and R_{1Z} profiles followed a theoretical square-law functional dependence [3]. The R_2^{QE} rates were found to be sensitive to osmotic pressure as well as the acyl position, thus yielding two important observations: enhanced transverse relaxation rates with increased amount of water per lipid, and limiting lower R_2^{QE} values as we dehydrate the membrane. The R_2^{QE} rates of the acyl segments and respective S_{CD} values tend to follow a square-law behavior [3] with increasing lipid dehydration. At higher hydration the square-law behavior is limited to those acyl segments deeper in the hydrophobic region, with a break as the head group is approached. These results clearly indicate that water enhances slow cooperative motions whereas they are suppressed by dehydration. Additional complementary Carr-Purcell-Meiboom-Gill (CPMG) dispersion measurements map the frequency dependence of relaxation rates. Such studies in presence of membrane proteins give insight into optimized lipid hydration for their biological functions.
[1] A. Leftin *et al.* (2011) *BBA* **1808**, 818-839.
[2] K.J. Mallikarjunaiah *et al*. (2011) *B.J*.**100**, 98-107.
[3] M.F. Brown (1982) *JCP***77**, 1576-1599.

423-Pos Board B192
Light Scattering on the Structural Characterization of DMPG Vesicles along the Bilayer Anomalous Phase Transition
Thais A. Enoki, M. Teresa Lamy, Vera B. Henriques.
University of São Paulo, São Paulo, Brazil.
Highly charged vesicles of the saturated anionic lipid dimyristoyl phosphatidylglycerol (DMPG) in low ionic strength medium exhibit a very peculiar thermo-structural behavior. Along a wide gel-fluid transition region, DMPG dispersions display several anomalous characteristics, like low turbidity, high electrical conductivity and viscosity. Here, static and dynamic light scattering (SLS and DLS) were used to characterize DMPG vesicles at different temperatures. Similar experiments were performed with the largely studied zwitterionic lipid dimyristoyl phosphatidylcholine (DMPC). SLS and DLS data yielded similar dimensions for DMPC vesicles at all studied temperatures. However, for DMPG, along the gel-fluid transition region, SLS indicated a threefold increase in the vesicle radius of gyration, whereas the hydrodynamic radius, as obtained from DLS, increased 30% only. Despite the anomalous increase in the radius of gyration, DMPG lipid vesicles maintain isotropy, since no light depolarization was detected. Hence, SLS data are interpreted regarding the presence of isotropic vesicles along the DMPG anomalous transition, but highly perforated vesicles, with large holes. DLS/SLS discrepancy along the DMPG transition region is discussed in terms of the interpretation of the Einstein-Stokes relation for porous vesicles. Therefore, SLS data are shown to be much more appropriate for measuring porous vesicle dimensions than the vesicle diffusion coefficient. Although the underlying microscopic process which leads to the opening of pores in charged DMPG bilayer is very intriguing and deserves further investigation, one could envisage biotechnological applications, with vesicles being produced to enlarge and perforate in a chosen temperature and/or pH value, for a desired drug delivery process.

424-Pos Board B193
Membrane Structure and Intermembrane Forces Observed with Small Angle X-Ray Scattering
Jacob J. Kinnun[1], K.J. Mallikarjunaiah[2], Luis A. Palacio[1], Michael F. Brown[2], Horia I. Petrache[1].
[1]Indiana University-Purdue University Indianapolis, Indianapolis, IN, USA, [2]University of Arizona, Tucson, AZ, USA.
Cellular functions rely on intermembrane interactions and forces that govern membrane structure and hence modulate lipid-protein interactions [1]. Moreover, the strengths of intermembrane forces vary with interlamellar distances. Here we address material properties of the membrane with structural deformation due to external stress using small-angle X-ray scattering (SAXS) spectroscopy. The SAXS technique has been extensively used to study membrane bilayers through application of osmotic pressure. However, distinguishing the effects of osmotic stress on intermembrane forces (separation force) and membrane deformation requires further investigation [2]. We subjected model membranes (DMPC) in the liquid-crystalline state to dehydration and high osmotic pressures (up to 25 MPa). The work of removal of water from the interlamellar region to the bulk water region restructures the membrane assembly and prompts us to examine membrane properties using complementary techniques. Using SAXS we were able to directly measure the interlamellar spacings and compare the results to solid-state ^{2}H NMR data [1,3]. We correlated the influences of dehydration and osmotic pressure in SAXS results through the interlamellar spacing. This approach allowed us to gauge the strength of intermembrane forces for a given hydration state. The combined techniques allowed us to estimate the area per lipid and structural deformation at the molecular level. Under high osmotic pressure or low hydration we found large area deformations up to 15% [1]. Temperature variation with this approach is used to discern entropic-based forces (lipid protrusions) and ordering-based forces (the hydration force). These findings show significant area deformation of membranes and provide insight into the forces that govern intermembrane interactions.
[1] K.J. Mallikarjunaiah *et al*. (2011) *B.J* **100**, 98-107.
[2] V.A. Parsegian *et al*. (1979) *PNAS* **76**, 2750-2754.
[3] H.I. Petrache and M.F. Brown (2007) *Meth. Mol. Biol*. **400**, 341-353.

425-Pos Board B194
Molecular Dynamics Simulation of Diacylglycerols in Phosphatidycholine Lipid Bilayers
Mohammad S. Alwarawrah, Juyang Huang.
Texas Tech University, Lubbock, TX, USA.
In this study, atomistic MD simulations were performed to investigate the interactions between diacylglycerols (i.e. DPG, POG, or DOG) and phosphatidylcholine (i.e. POPC or DOPC) bilayers. Our results show that diacylglycerols (DAG) increase acyl chain order, headgroup spacing and bilayer thickness, and reduce area-per-lipid. In a lipid bilayer, in order to avoid the unfavorable exposure of DAG hydrophobic parts to water, neighboring phospholipid (PC) headgroups move toward DAG to provide cover. This interaction between DAG and phospholipid is explained by the Umbrella Model. Comparing the three types of DAG in POPC and DOPC bilayers, DOG is located closer to the bilayer/aqueous interfaces than DPG and POG and it requires more coverage according to our umbrella index calculation, likely due to its longer and